

chain nodes :

1 2 3 4 12 13

ring nodes :

5 6 7 8 9 10 15 16 17 18 19 20

chain bonds :

1-12 1-2 2-3 2-4 3-13 3-16 5-19

ring bonds :

5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds :

1-2 2-3 2-4 3-16

exact bonds :

1-12 3-13 5-19

normalized bonds :

5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20

isolated ring systems :

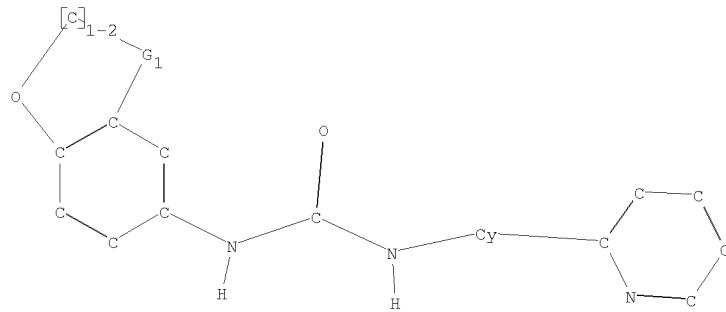
containing 15 :

G1:C,O

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

Match level :

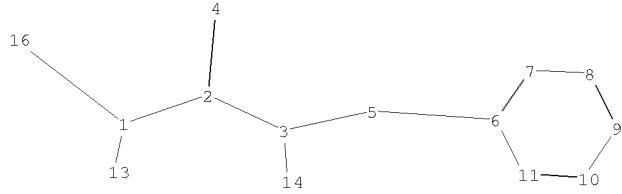
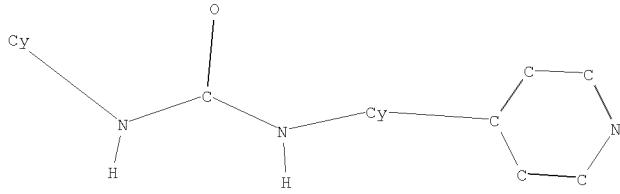
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS  
13:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom



chain nodes :  
 10 11 12 13 14 24 25  
 ring nodes :  
 1 2 3 4 5 6 7 8 9 15 16 17 18 19 20  
 chain bonds :  
 6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-15  
 ring bonds :  
 1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-16 15-20 16-17 17-18 18-19 19-20  
 exact/norm bonds :  
 3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-15  
 normalized bonds :  
 1-2 1-6 2-3 5-6 15-16 15-20 16-17 17-18 18-19 19-20  
 isolated ring systems :  
 containing 1 : 15 :

G1:C,O

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS  
 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS  
 25:CLASS  
 Generic attributes :  
 14:  
 Saturation : Unsaturated  
 Number of Carbon Atoms : less than 7  
 Number of Hetero Atoms : Exactly 1

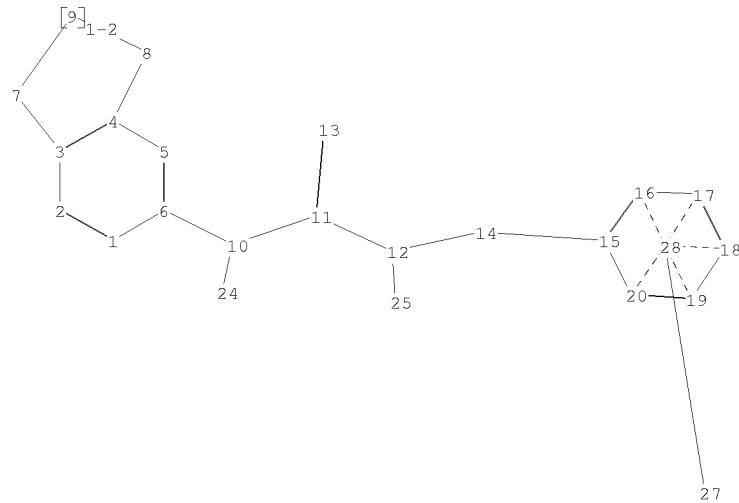
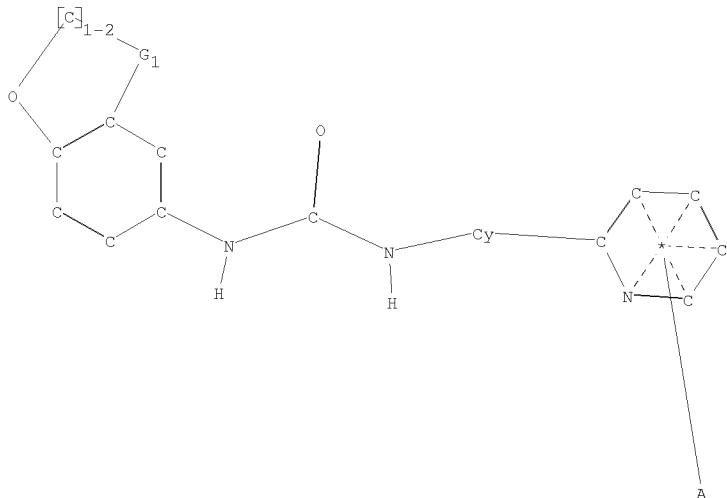


chain nodes :  
 1 2 3 4 5 13 14 16  
 ring nodes :  
 6 7 8 9 10 11  
 chain bonds :  
 1-13 1-2 1-16 2-3 2-4 3-5 3-14 5-6  
 ring bonds :  
 6-11 6-7 7-8 8-9 9-10 10-11  
 exact/norm bonds :  
 1-2 1-16 2-3 2-4 3-5 5-6  
 exact bonds :  
 1-13 3-14  
 normalized bonds :  
 6-11 6-7 7-8 8-9 9-10 10-11

G1:C,O

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

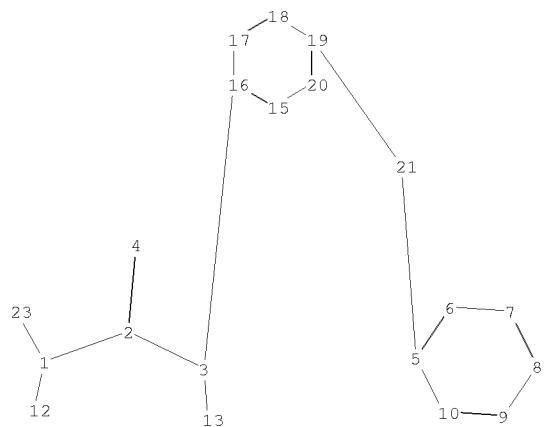
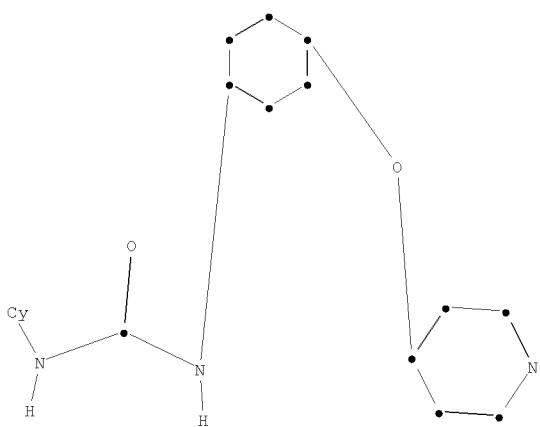
Match level :  
 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
 13:CLASS 14:CLASS 16:Atom  
 Generic attributes :  
 5:  
 Saturation : Unsaturated  
 Number of Hetero Atoms : Exactly 1



chain nodes :  
 10 11 12 13 14 24 25 27  
 ring nodes :  
 1 2 3 4 5 6 7 8 9 15 16 17 18 19 20  
 chain bonds :  
 6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-15  
 ring bonds :  
 1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-16 15-20 16-17 17-18 18-19 19-20  
 exact/norm bonds :  
 3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-15  
 normalized bonds :  
 1-2 1-6 2-3 5-6 15-16 15-20 16-17 17-18 18-19 19-20  
 isolated ring systems :  
 containing 1 : 15 :

G1:C,O

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS  
 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS  
 25:CLASS 27:CLASS 28:CLASS  
 Generic attributes :  
 14:  
 Saturation : Unsaturated  
 Number of Carbon Atoms : less than 7  
 Number of Hetero Atoms : Exactly 1

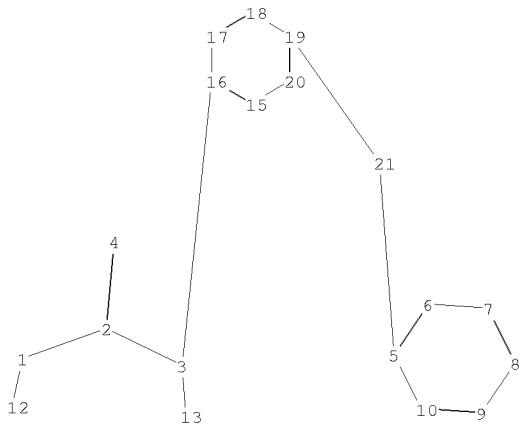
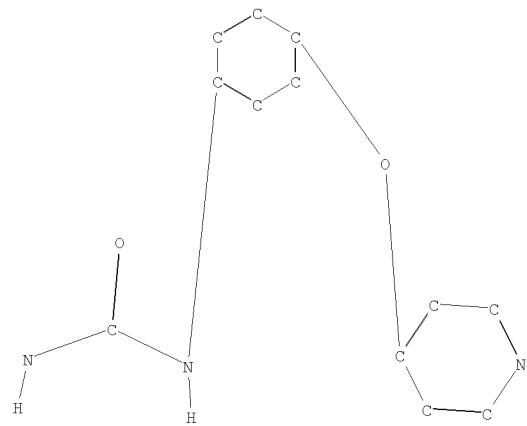


chain nodes :  
 1 2 3 4 12 13 21 23  
 ring nodes :  
 5 6 7 8 9 10 15 16 17 18 19 20  
 chain bonds :  
 1-12 1-2 1-23 2-3 2-4 3-13 3-16 5-21 19-21  
 ring bonds :  
 5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20  
 exact/norm bonds :  
 1-2 1-23 2-3 2-4 3-16 5-21 19-21  
 exact bonds :  
 1-12 3-13  
 normalized bonds :  
 5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20  
 isolated ring systems :  
 containing 15 :

G1:C,O

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

Match level :  
 1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS  
 13:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS 23:Atom  
 Generic attributes :  
 23:  
 Number of Carbon Atoms : 7 or more  
 Type of Ring System : Polycyclic



chain nodes :

1 2 3 4 12 13 21

ring nodes :

5 6 7 8 9 10 15 16 17 18 19 20

chain bonds :

1-12 1-2 2-3 2-4 3-13 3-16 5-21 19-21

ring bonds :

5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds :

1-2 2-3 2-4 3-16 5-21 19-21

exact bonds :

1-12 3-13

normalized bonds :

5-10 5-6 6-7 7-8 8-9 9-10 15-16 15-20 16-17 17-18 18-19 19-20

isolated ring systems :

containing 15 :

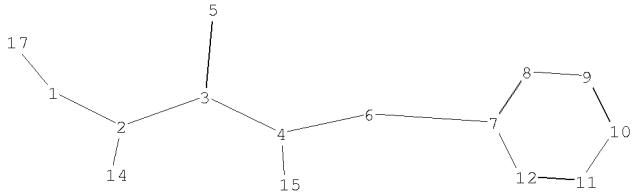
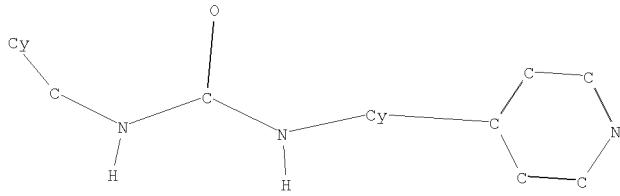
G1:C,O

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 12:CLASS

13:CLASS 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 21:CLASS



chain nodes :

1 2 3 4 5 6 14 15 17

ring nodes :

7 8 9 10 11 12

chain bonds :

1-2 1-17 2-3 2-14 3-4 3-5 4-6 4-15 6-7

ring bonds :

7-12 7-8 8-9 9-10 10-11 11-12

exact/norm bonds :

1-2 1-17 2-3 3-4 3-5 4-6 6-7

exact bonds :

2-14 4-15

normalized bonds :

7-12 7-8 8-9 9-10 10-11 11-12

G1:C,O

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

Match level :

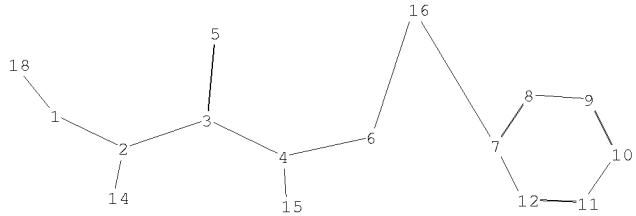
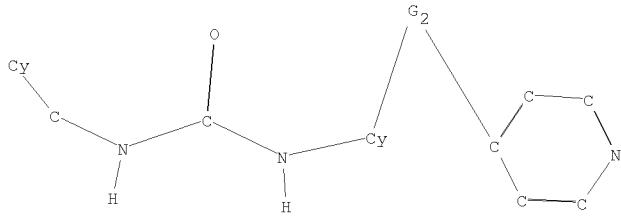
1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
12:Atom 14:CLASS 15:CLASS 17:Atom

Generic attributes :

6:

Saturation : Unsaturated

Number of Hetero Atoms : Exactly 1



chain nodes :  
 1 2 3 4 5 6 14 15 16 18

ring nodes :  
 7 8 9 10 11 12

chain bonds :  
 1-2 1-18 2-3 2-14 3-4 3-5 4-6 4-15 6-16 7-16

ring bonds :  
 7-12 7-8 8-9 9-10 10-11 11-12

exact/norm bonds :  
 1-2 1-18 2-3 3-4 3-5 4-6 6-16 7-16

exact bonds :  
 2-14 4-15

normalized bonds :  
 7-12 7-8 8-9 9-10 10-11 11-12

G1:C,O

G2:O,S,N,CH3,Et,n-Pr,MeO,EtO,n-PrO

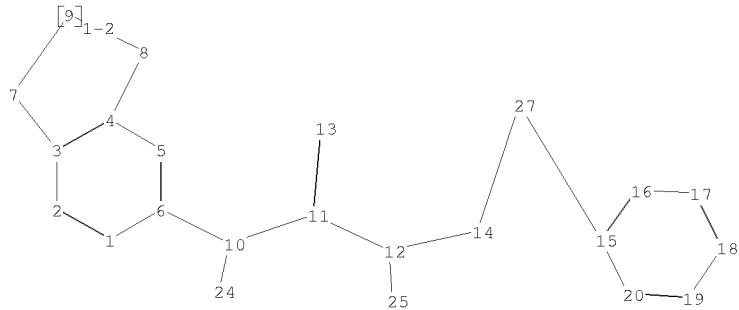
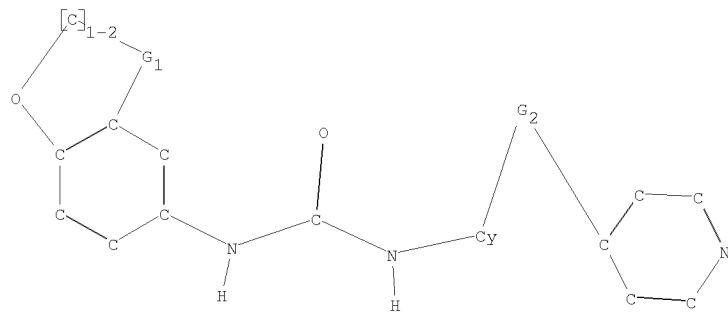
Match level :  
 1:Atom 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom 11:Atom  
 12:Atom 14:CLASS 15:CLASS 16:CLASS 18:Atom

Generic attributes :

6:

Saturation : Unsaturated

Number of Hetero Atoms : Exactly 1



chain nodes :  
 10 11 12 13 14 24 25 27

ring nodes :  
 1 2 3 4 5 6 7 8 9 15 16 17 18 19 20

chain bonds :  
 6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-27 15-27

ring bonds :  
 1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-20 15-16 16-17 17-18 18-19 19-20

exact/norm bonds :  
 3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-27 15-27

normalized bonds :  
 1-2 1-6 2-3 5-6 15-20 15-16 16-17 17-18 18-19 19-20

isolated ring systems :  
 containing 1 : 15 :

G1:C,O

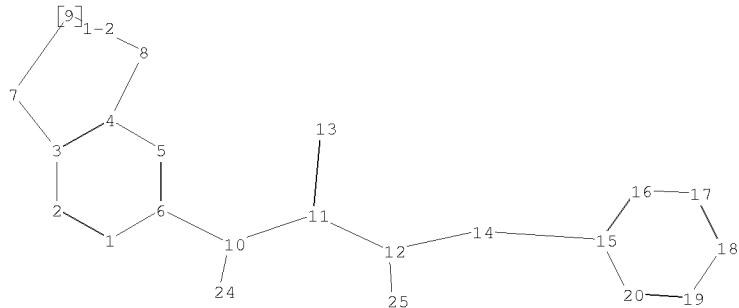
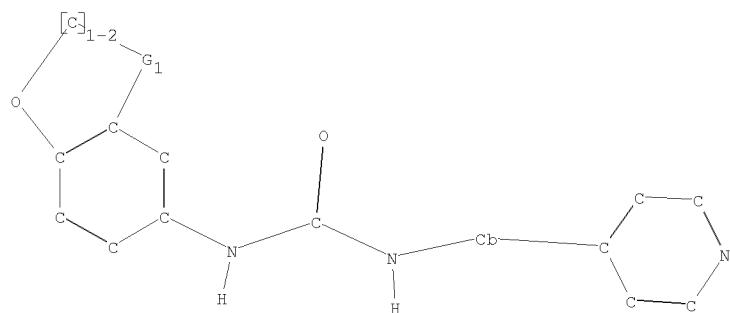
G2:O,S,N,CH<sub>3</sub>,Et,n-Pr,MeO,EtO,n-PrO

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS  
 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS  
 25:CLASS 27:CLASS

Generic attributes :

14:  
 Saturation : Unsaturated  
 Number of Hetero Atoms : Exactly 1



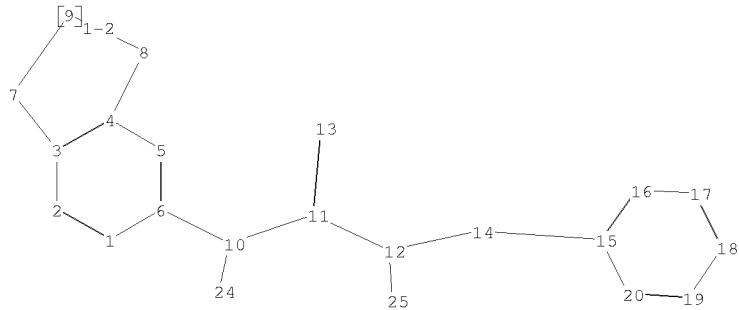
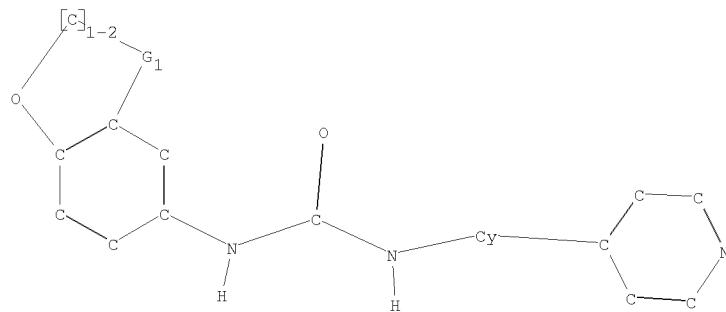
```

chain nodes :
 10 11 12 13 14 24 25
ring nodes :
 1 2 3 4 5 6 7 8 9 15 16 17 18 19 20
chain bonds :
 6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-15
ring bonds :
 1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-16 15-20 16-17 17-18 18-19 19-20
exact/norm bonds :
 3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-15
normalized bonds :
 1-2 1-6 2-3 5-6 15-16 15-20 16-17 17-18 18-19 19-20
isolated ring systems :
 containing 1 : 15 :

```

G1;C, O

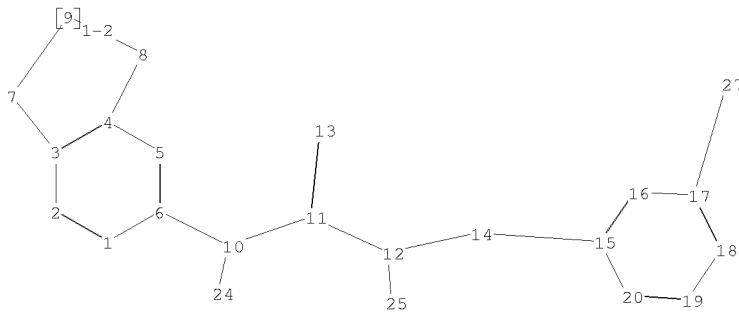
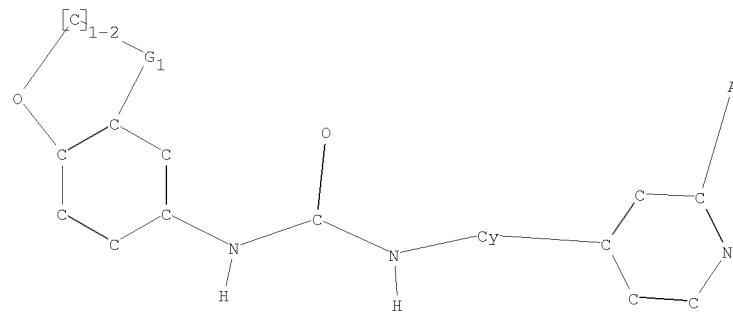
Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS  
12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS  
25:CLASS



chain nodes :  
 10 11 12 13 14 24 25  
 ring nodes :  
 1 2 3 4 5 6 7 8 9 15 16 17 18 19 20  
 chain bonds :  
 6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-15  
 ring bonds :  
 1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-16 15-20 16-17 17-18 18-19 19-20  
 exact/norm bonds :  
 3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-15  
 normalized bonds :  
 1-2 1-6 2-3 5-6 15-16 15-20 16-17 17-18 18-19 19-20  
 isolated ring systems :  
 containing 1 : 15 :

G1:C,O

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS  
 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS  
 25:CLASS  
 Generic attributes :  
 14:  
 Saturation : Unsaturated  
 Number of Carbon Atoms : less than 7  
 Number of Hetero Atoms : Exactly 1



chain nodes :  
 10 11 12 13 14 24 25 27

ring nodes :  
 1 2 3 4 5 6 7 8 9 15 16 17 18 19 20

chain bonds :  
 6-10 10-11 10-24 11-12 11-13 12-14 12-25 14-15 17-27

ring bonds :  
 1-2 1-6 2-3 3-4 3-7 4-5 4-8 5-6 7-9 8-9 15-16 15-20 16-17 17-18 18-19 19-20

exact/norm bonds :  
 3-4 3-7 4-5 4-8 6-10 7-9 8-9 10-11 10-24 11-12 11-13 12-14 12-25 14-15 17-27

normalized bonds :  
 1-2 1-6 2-3 5-6 15-16 15-20 16-17 17-18 18-19 19-20

isolated ring systems :  
 containing 1 : 15 :

G1:C,O

Match level :  
 1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS  
 12:CLASS 13:CLASS 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:Atom 20:Atom 24:CLASS  
 25:CLASS 27:CLASS

Generic attributes :

14:  
 Saturation : Unsaturated  
 Number of Carbon Atoms : less than 7  
 Number of Hetero Atoms : Exactly 1